# Supplementary material

## Synthesis details and structural characterization:

### 1. Acyl chloride synthesis:

Synthesis of 3,5-dinitrobenzoyl chloride (**1**). Following the described general procedure for the acyl chloride synthesis, 500 mg (2.36mmol) of 3,5-dinitrobenzoic acid in 4.5 mL of thionyl chloride were refluxed for 12 h. This yielded a white-yellowish solid that was used without further treatment.

Synthesis of benzoyl chloride (**2**). Following the described general procedure for the acyl chloride synthesis, 61 mg of benzoic acid (0.5mmol) in 2.5 mL of thionyl chloride were refluxed for 12 h. This yielded a white-yellowish solid that was used without further treatment.

### 2. Amide synthesis:

Synthesis of (3,5-dinitrophenyl)-piperidin-1-yl-methanone (**a1**). Following the described general procedure for the amide synthesis, 254mg (1.1mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 187 mg (2.2mmol) of piperidine and 304mg (2.2mmol) of K2CO3. The compound was a white/yellowish solid. Yield=57%. 1H NMR (400 MHz, CDCl3) δ 9.08 (t, J = 2.1 Hz, 1H), 8.58 (d, J = 2.2 Hz, 2H), 3.76 (s, 2H), 3.35 (s, 2H), 1.74 (s, 4H), 1.59 (s, 2H). 13C NMR (101 MHz, CDCl3) δ 165.24, 148.59, 139.91, 127.43, 119.57, 49.11, 43.80, 26.65, 25.49, 24.36. m/z calculated for 280.09280, found: 280.11 (M+H+).

Synthesis of (3,5-dinitrophenyl)-piperazin-1-yl-methanone (**a2**). Following the described general procedure for the amide synthesis, 461 mg (2 mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 345mg (4 mmol) of piperazine and 553 mg (4 mmol) of K2CO3. The product was used directly in the synthesis of **a8**.

Synthesis of (3,5-dinitrophenyl)-4-hydroxypiperidin-1-yl-methanone (**a3**). Following the described general procedure for the amide synthesis, 254 mg (1.1mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 223mg (2.2mmol) of 4-hydroxypiperidine and 254mg (2.2mmol) of K2CO3. The compound was a white/yellowish solid. Yield=52%. 1H NMR (400 MHz, CDCl3): δ 9.09 (t, J = 2.2 Hz, 1H), 8.59 (d, J = 2.1 Hz, 2H), 4.08 (m, 2H), 3.62 (s, 2H), 3.29 (d, J = 11.6 Hz, 1H), 2.01 (s, 1H), 1.88 (s, 1H), 1.74 (s, 2H), 1.59 (s, 1H). 13C NMR (101 MHz, CDCl3) δ 165.38, 148.63, 139.50, 127.44, 119.78, 66.24, 44.98, 39.74, 34.06, 33.54. m/z calculated for 296.08771, found: 296.08 (M+H+).

Synthesis of (3,5-dinitrophenyl)(morpholino)methanone (**a4**). Following the described general procedure for the amide synthesis, 161 mg (0.7mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 122 mg (1.4 mmol) of morpholine and 194 mg (1.4 mmol) of K2CO3. The compound was a white solid. Yield=88%. 1H NMR (400 MHz, CDCl3): δ 9.09 (t, J = 2.3 Hz, 1H), 8.60 (d, J = 2.2 Hz, 2H), 3.83 (s, 4H), 3.69 (s, 2H), 3.46 (s, 2H). 13C NMR (101 MHz, CDCl3) δ 165.38, 148.67, 138.76, 127.67, 119.99, 66.71, 48.35, 43.03. m/z calculated for 282.07206, found: 282.04 (M+H+).

Synthesis of (3,5-dinitrophenyl)-4-benzylpiperazin-1-yl-methanone (**a5**). Following the described general procedure for the amide synthesis, 161mg (0.7mmol) of compound **1** was dissolved in ethyl acetate (4 mL) and was added to a solution in ethyl acetate (4 mL) of 159mg (0.9 mmol) of 4-benzylpiperazine and 415mg (3mmol) of K2CO3. The compound was a white solid. Yield=88%. 1H NMR (400 MHz, DMSO-d6) δ 8.85 (t, J = 2.2 Hz, 1H), 8.61 (d, J = 2.1 Hz, 2H), 7.38 – 7.19 (m, 6H), 3.66 (t, J = 5.1 Hz, 2H), 3.52 (s, 58 2H), 3.33 (br s, 2H), 2.47 (d, J = 5.1 Hz, 2H), 2.36 (t, J = 5.2 Hz, 2H). 13C NMR (101 MHz, DMSO-d6) δ 164.74, 148.17, 138.87, 137.78, 128.93, 128.26, 127.55, 127.10, 119.15, 61.74, 52.44, 51.77, 47.10, 41.87. m/z calculated for 371.13500, found: 370.85 (M+H+).

Synthesis of (3,5-dinitrophenyl)-4-benzylpiperidin-1-yl-methanone (**a6**). Following the described general procedure for the amide synthesis, 254mg (1.1mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 386 mg (2.2mmol) of 4-benzylpiperidine and 304mg (2.2mmol) of K2CO3. The compound was a white solid. Yield=53%. 1H NMR (400 MHz, CDCl3): δ 9.08 (t, J = 2.1 Hz, 1H), 8.58 (d, J = 2.1 Hz, 2H), 7.30 (t, J = 7.4 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.15 (d, 2H), 4.70 (d, J = 13.3 Hz, 1H), 3.57 (d, J = 13.5 Hz, 1H), 3.11 (t, J = 13.2 Hz, 1H), 2.81 (t, J = 12.9 Hz, 1H), 2.61 (t, J = 6.5 Hz, 2H), 1.91-1.79 (m, J = 12.0, 8.0, 4.0 Hz, 2H), 1.69 (d, J = 13.2 Hz, 1H), 1.36 (d, J = 13.1 Hz, 1H), 1.21 (d, J = 13.4 Hz, 1H). 13C NMR (101 MHz, CDCl3) δ 165.25, 148.60, 139.81, 139.56, 129.18, 128.56, 127.45, 126.40, 119.64, 48.40, 43.13, 42.86, 38.22, 32.69, 31.63. m/z calculated for 370.13975, found: 370.31 (M+H+).

Synthesis of 4-(3,5-dinitrobenzoyl)-1,1-dimethylpiperazin-1-ium (**a8**). Following the synthesis of compound **a2**, the unpurified product **a2** and 304mg (2.2 mmol) of K2CO3 were dissolved in 5 mL of MeCN. Then 0.64mL (2mmol) of CH3I were added to the mixture and the reaction was heated up to 60°C. After 2h, the reaction was stopped, the solid was filtered off and the MeCN was evaporated under reduced pressure. Then, the solid was recrystalized in acetone, yielding the final product **a8**. The compound was an orange solid. Yield=33%. 1H NMR (400 MHz, DMSO-d6) δ 8.91 (t, J = 2.5 Hz, 1H), 8.65 (s, 2H), 4.00 (s, 2H), 3.69 (s, 2H), 3.55 (s, 2H), 3.44 (s, 2H), 3.19 (s, 6H). 13C NMR (101 MHz, DMSO-d6) δ 165.18, 148.32, 137.59, 127.67, 119.60, 59.71, 50.66, 36.10. m/z calculated for 309,11935, found: 309.02 (M+H+).

Synthesis of N-(2-hydroxyethyl)-3,5-dinitrobenzamide (**b1**). Following the described general procedure for the amide synthesis, 543.5mg (2.4 mmol) of compound **1** was dissolved in ethyl acetate (7 mL) and was added to a solution in ethyl acetate (7 mL) of 610 mg (10mmol) of 2-aminoethan-1-ol. No K2CO3 was added. The compound was a yellow solid. Yield=40%. 1H NMR 1H NMR (400 MHz, CDCl3) δ 8.98 (dt, J = 13.9, 2.1 Hz, 3H), 3.61 (t, J = 5.2 Hz, 2H), 3.48 – 3.36 (m, 2H). 13C NMR (101 MHz, CDCl3): δ 163.71, 148.43, 137.71, 127.55, 120.74, 60.38, 42.75. m/z calculated for 256.05641, found: 256.08 (M+H+).

Synthesis of N-(3-hydroxypropyl)-3,5-dinitrobenzamide (**b2**). Following the described general procedure for the amide synthesis, 648mg (2.8 mmol) of compound **1** was dissolved in ethyl acetate (10 mL) and was added to a solution in ethyl acetate (10 mL) of 421 mg (5.6mmol) of 3-aminopropan-1-ol and 774mg (5.6mmol) of K2CO3. The compound was a white solid. Yield=50%. 1H NMR (400 MHz, DMSO-d6): δ 9.16 (t; J = 5.4 Hz; 1H; H-8), 9.04 (m; 2H), 8.94 (t; J = 2.2 Hz; 1H), 4.51 (t; J = 5.1 Hz; 1H), 3.48 (q; J = 6.0 Hz; 2H), 3.38 (q, J = 6.7 Hz, 2H), 1.72 (p, J = 6.6 Hz, 2H; H-10). 13C NMR (101 MHz, DMSOd6): δ 162.00, 148.19, 137.11, 127.46, 120.73, 58.47, 37.09, 32.08. m/z calculated for 270.07206, found: 269.99 (M+H+).

Synthesis of N-(5-hydroxypentyl)-3,5-dinitrobenzamide (**b3**). Following the described general procedure for the amide synthesis, 600mg (2.6 mmol) of compound **1** was dissolved in ethyl acetate (10 mL) and was added to a solution in ethyl acetate (10 mL) of 537 mg (5.2mmol) of 5-aminopentan-1-ol and 724mg (5.2mmol) of K2CO3. The compound was a white/yellowish solid. Yield=78%. 1H NMR (400 MHz, DMSO-d6): δ 9.17 (t; J = 5.8 Hz; 1H), 9.06 (d; J = 2.1 Hz; 2H), 8.95 (t; J = 2.1 Hz; 1H), 4.39 (t; J = 5.1 Hz; 1H), 3.40 (q; J = 6.0 Hz; 2H), 3.32 (t; J = 6.4 Hz; 2H), 1.57 (p; J = 7.2 Hz; 2H), 1.46 (p; J = 6.6 Hz; 2H), 1.35 (tt; J = 8.6, 5.2 Hz; 2H). 13C NMR (101 MHz, DMSO-d6): δ 161.92, 148,22, 137.10, 127.47, 120.76, 60.62, 39,79, 32.23, 28.71, 23.07. m/z calculated for 298.10336, found: 298.01 (M+H+).

Synthesis of 2-(3,5-dinitrobenzamido)ethyl 3,5-dinitrobenzoate (**c1**). Following the described general procedure for the amide synthesis, 208mg (0.9 mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 20 mg (0.3mmol) of 2-aminoethan-1-ol and 110mg (0.8mmol) of K2CO3. The compound was a white solid. Yield=39%. 1H NMR (300 MHz, DMSO-d6): δ 9.07-8.91 (m, 6H), 4.57 (t, J = 5.3 Hz, 2H), 3.80 (q, J=5.4 Hz, 2H).

Synthesis of 5-(3,5-dinitrobenzamido)pentyl 3,5-dinitrobenzoate (**c2**). Following the described general procedure for the amide synthesis, 208mg (0.9 mmol) of compound **1** was dissolved in ethyl acetate (5 mL) and was added to a solution in ethyl acetate (5 mL) of 40 mg (0.4mmol) of 5-aminopentan-1-ol and 111mg (0.8mmol) of K2CO3. The compound was a white solid. Yield=46%. 1H NMR (400 MHz, DMSO-d6) δ 9.20 (t, J = 5.6 Hz, 1H), 9.05-9.00 (m, J = 2.7, 1.2 Hz, 3H), 8.94 (t, J = 1.8 Hz, 1H), 8.88 (d, J = 2.1 Hz, 2H), 4.42 (t, J = 6.5 Hz, 2H), 3.38 (t, J = 6.3 Hz, 2H), 1.83 (p, J = 6.9 Hz, 2H), 1.66 (p, J = 7.2 Hz, 2H), 1.55 – 1.44 (m, 2H). 13C NMR (101 MHz, DMSO-d6) δ 162.67, 162.05, 148.45, 148.26, 137.13, 132.81, 128.87, 127.51, 122.57, 120.82, 66.35, 39.55, 28.44, 27.73, 22.91. m/z calculated for 492.09973, found: 492.06 (M+H+).

Synthesis of product N-(4-methoxyphenyl)-3,5-dinitrobenzamide (**f1**). Following the described general procedure for the amide synthesis, compound **1** was dissolved in ethyl acetate and was added to a solution of 4-methoxyaniline and K2CO3. The compound was a yellow solid. Yield=31%. 1H NMR (400 MHz, DMSO-d6) δ 10.74 (s, 1H), 9.15 (t, J = 1.9 Hz, 2H), 8.97 (s, 1H), 7.68 (d, J = 7.2 Hz, 2H), 6.96 (d, J = 7.3 Hz, 2H), 3.76 (s, 3H). 13C NMR (101 MHz, DMSO-d6) δ 160.78, 156.16, 148.15, 137.52, 131.30, 127.93, 122.31, 120.99, 113.91, 55.24, 30.73. m/z calculated for 318.07206, found: 318.01 (M+H+).

### 3. Mitsunobu reaction:

Synthesis of (3,5-dinitrophenyl)(4-(4-methoxyphenoxy)piperidin-1-yl)methanone (**a7**). Following the described general procedure for the Mitsunobu reaction, 224mg (0.85mmol) of PPh3 in 2mL of DCM was added to a solution in 2mL of DCM of 42mg (0.34mmol) of 4-methoxyphenol, 215mg (0.85mmol) of ADDP and 100mg (0.34mmol) of **a3**. The compound was a yellow solid. Yield=29%. 1H NMR (400 MHz, CDCl3) δ 9.09 (t, J = 1.4 Hz, 1H), 8.64 – 8.57 (m, 2H), 6.85 (q, J = 9.2 Hz, 4H), 4.52 (p, J = 4.6 Hz, 1H), 3.98 (s, 1H), 3.84 (s, 1H), 3.77 (d, J = 1.0 Hz, 3H), 3.69 (s, 1H), 3.37 (s, 1H), 2.01 (s, 1H), 1.87 (s, 2H). 13C NMR (101 MHz, CDCl3) δ 162.85, 159.15, 148.72, 138.26, 129.54, 127.27, 121.11, 120.61, 114.55, 67.90, 40.96, 29.55, 29.37, 27.05, 26.13. m/z calculated for 402.12958, found: 402.02 (M+H+).

Synthesis of N-(3-(4-methoxyphenoxy)propyl)-3,5-dinitrobenzamide (**d1**). Following the described general procedure for the Mitsunobu reaction, 223mg (0.85mmol) of PPh3 in 2mL of DCM was added to a solution in 2mL of DCM of 42mg (0.34mmol) of 4-methoxyphenol, 215mg (0.85mmol) of ADDP and 92mg (0.32mmol) of **b2**. In this reaction a secondary product also formed (**e2**), and to separate both compounds a second column was required (eluent 100% toluene to 96% toluene /4% EtOAc). The compound was an orange solid. Yield=42%. 1H NMR (400 MHz, CDCl3) δ 9.09 (t, J = 2.2 Hz, 1H), 8.99 (d, J = 2.1 Hz, 2H), 6.84 – 6.74 (q, J = 6.40, 6.29, 6.29 Hz, 4H), 4.04 (t, J = 5.7 Hz, 2H), 3.71 (s, 3H), 3.64 (t, J = 6.5 Hz, 2H), 2.09 (p, J = 6.1 Hz, 2H). 13C NMR (101 MHz, CDCl3) δ 163.30, 154.42, 152.83, 148.90, 138.32, 127.78, 121.24, 115.66, 115.14, 67.43, 56.09, 38.95, 28.93. m/z calculated for 376.11393, found: 375.97 (M+H+).

Synthesis of N-(5-(4-methoxyphenoxy)pentyl)-3,5-dinitrobenzamide (**d2**). Following the described general procedure for the Mitsunobu reaction, 223mg (0.85mmol) of PPh3 in 2mL of DCM was added to a solution in 2mL of DCM of 42mg (0.34mmol) of 4-methoxyphenol, 215mg (0.85mmol) of ADDP and 100mg (0.34mmol) of **b3**. The compound was an orange/yellowish solid. Yield=43%. 1H NMR (400 MHz, CDCl3) δ 9.14 (s, 1H), 8.94 (t, J = 1.6 Hz, 2H), 6.80 (s, 4H), 6.63 (br s, 1H), 3.93 (t, J = 6.1 Hz, 2H), 3.75 (s, 3H), 3.57 (q, J = 6.6 Hz, 2H), 1.83 (p, J = 6.6 Hz, 2H), 1.75 (q, J = 7.4 Hz, 2H), 1.61 (q, J = 7.8 Hz, 2H). 13C NMR: (101 MHz, CDCl3) δ 162.89, 153.91, 148.72, 138.19, 127.27, 121.12, 115.48, 114.76, 68.33, 40.82, 29.16, 29.01, 23.75. m/z calculated for 404.14523, found: 404.11 (M+H+).

Synthesis of 2-(3,5-dinitrophenyl)-4,5-dihydrooxazole (**e1**). Trying to react **b1** with 4-methoxyphenol using the described general procedure for the Mitsunobu reaction led to the formation of only the intramolecular cyclization product. For this, 224mg (0.85mmol) of PPh3 in 2mL of DCM was added to a solution in 2mL of DCM of 42mg (0.34mmol) of 4-methoxyphenol, 215mg (0.85mmol) of ADDP and 82mg (0.34mmol) of **b1**. The compound was a white-yellowish solid. Yield=70%. 1H NMR (400 MHz, DMSO-d6): δ 8.88 (m; 1H), 8.75 (m; 2H), 4.49 (t; J = 9.6 Hz; 2H), 4.01 (t; J = 9.6 Hz; 2H). 13C NMR (101 MHz, DMSO-d6): δ 160.19, 148.41, 130.18, 127.41, 120.95, 68.83, 54.86. m/z calculated for 238.04585, found: 238.02 (M+H+).

Synthesis of 2-(3,5-dinitrophenyl)-5,6-dihydro-4H-1,3-oxazine (**e2**). This compound was isolated from the same reaction of the synthesis of **d1**. Yield=15%. 1H NMR (400 MHz, DMSO-d6): δ 8.89 (t; J = 2.2 Hz; 1H), 8.83 (d; J = 2.2 Hz; 2H), 4.45 (t; J = 5.4 Hz; 2H), 3.59 (t; J = 5.8 Hz; 2H), 1.95 (p; J = 5.6 Hz; 2H). 13C NMR (101 MHz, DMSO-d6): δ 150.99, 148.21, 136.61, 126.14, 119.93, 65.79, 42.23, 21.18. m/z calculated for 252.06150, found: 252.01 (M+H+).

### 4. Diamide formation:

Synthesis of N-(5-chloropentyl)-3,5-dinitrobenzamide (**3**). Following the first step described in the general procedure for the diamide formation, 298mg (1mmol) of **b3** was dissolved in toluene/SOCl2 (1/1 in volume, total volume 2,9mL), and 0,1 mL of DMF was added to the reaction mixture. The compound was a white solid. Yield=97%. 1H NMR (400 MHz, CDCl3) δ 9.16 (t, J = 2.2 Hz, 1H), 8.96 (d, J = 2.1 Hz, 2H), 6.60 (t, J = 5.8 Hz, 1H), 3.56 (dt, J = 9.0, 6.5 Hz, 4H), 1.85 (p, J = 6.7 Hz, 2H), 1.72 (p, J = 7.3 Hz, 2H), 1.58 (tt, J = 9.7, 5.8 Hz, 2H). 13C NMR (101 MHz, CDCl3) δ 162.93, 148.77, 138.13, 127.76, 121.21, 44.91, 40.68, 32.05, 28.81, 24.25.

Synthesis of N-(5-azidopentyl)-3,5-dinitrobenzamide (**4**). Following the second step described in the general procedure for the diamide formation, 316mg (0.97mmol) of compound **3**, 45mg (0.3mmol) of NaI and 195mg (3mmol) of NaN3 were dissolved in 10mL of MeCN. The compound was a yellow oil. Mass of product obtained: 311mg. Yield=97%. 1H NMR (400 MHz, CDCl3) δ 9.18 (t, J = 2.0 Hz, 1H), 8.96 (dd, J = 2.2, 1.0 Hz, 2H), 6.48 (br s, 1H), 3.56 (q, J = 6.8 Hz, 2H), 3.33 (t, J = 6.6 Hz, 2H), 1.70 (dp, J = 18.0, 7.7 Hz, 4H), 1.51 (p, J = 7.7 Hz, 2H).

Synthesis of N-(5-aminopentyl)-3,5-dinitrobenzamide (**5**). Following the third step described in the general procedure for the diamide formation, 0.94mmol of compound **4** and 500mg (1.9mmol) of PPh3 were dissolved in 6mL of THF. After 24h, 0.1mL of distilled water was added to the mixture, and the reaction was stirred for another 24h. After the end of the reaction, the solvent was evaporated and the product used without further purification.

Synthesis of N,N'-(pentane-1,5-diyl)bis(3,5-dinitrobenzamide) (**c3**). Following the described general procedure for the amide synthesis, 217mg (0.94mmol) of compound **1** dissolved in ethyl acetate (10 mL) was added to a solution in ethyl acetate (15 mL) of 278 mg (0.94mmol) of compound **5** and 304mg (2.2mmol) of K2CO3. The compound was a white solid. Yield=14%. 1H NMR (400 MHz, DMSO-d6): δ 9.19 (t; J = 5.6 Hz; 2H), 9.03 (d; J = 2.0 Hz; 4H), 8.94 (t; J = 2.1 Hz; 2H), 3.33 (d; J = 5.9 Hz; 4H), 1.62 (p; J = 7.2 Hz; 4H), 1.41 (d; J = 7.2 Hz; 2H). 13C NMR (101 MHz, DMSO-d6) δ 162.67, 162.05, 148.45, 148.26, 137.13, 132.81, 128.87, 127.51, 122.57, 120.82, 66.35, 39.55, 28.44, 27.73, 22.91. m/z calculated for 491.11572, found: 491.01 (M+H+).

Synthesis of N-(5-benzamidopentyl)-3,5-dinitrobenzamide) (**c4**). Following the described general procedure for the amide synthesis, 61mg (0.5mmol) of compound **2** dissolved in ethyl acetate (7 mL) was added to a solution in ethyl acetate (10 mL) of 148 mg (0.5mmol) of compound **5** and 138mg (1mmol) of K2CO3. The compound was a white solid. Yield=55%. 1H NMR (400 MHz, CDCl3) δ 9.04 (s, 3H), 7.55 (m, 3H), 7.44 (t, J = 7.1 Hz, 1H), 7.32 (t, J = 7.6 Hz, 2H), 6.28 (s, 1H), 3.54 (m, Hz, 4H), 1.81 (p, J = 6.6 Hz, 2H), 1.69 (p, J = 6.6 Hz, 2H), 1.50 (p, J = 6.9 Hz, 2H). 13C NMR (101 MHz, DMSO-d6) δ 169.38, 163.45, 150.83, 131.76, 128.73, 127.73, 126.63, 120.79, 40.45, 38.83, 29.67, 27.59, 23.18. m/z calculated for 401.14556, found: 401.17 (M+H+).